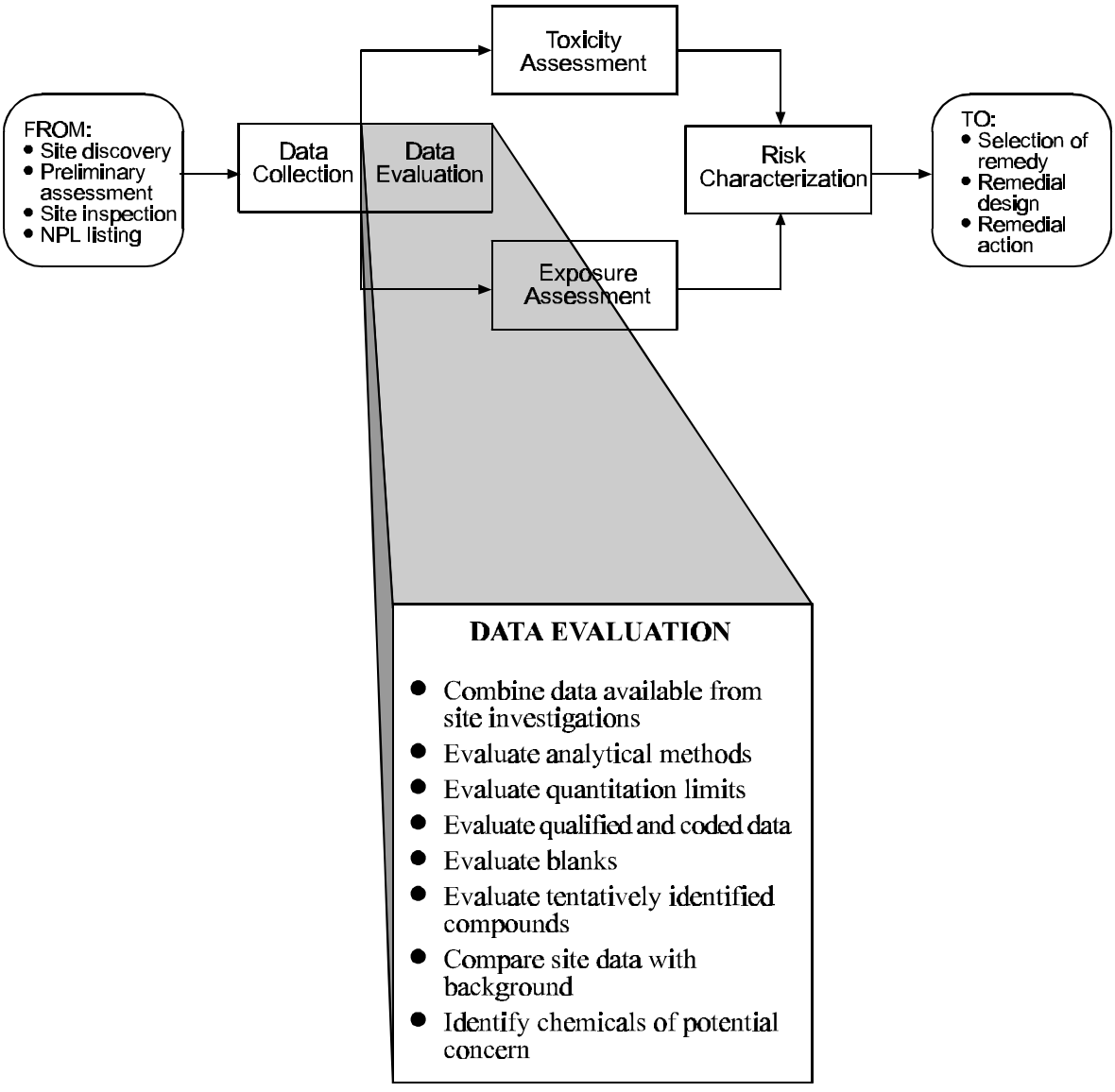
CHAPTER 5
DATA EVALUATION



CHAPTER 5

DATA EVALUATION

After a site sampling investigation has been completed (see Chapter 4), a large quantity of analytical data is usually available. Each sample may have been analyzed for the presence of over one hundred chemicals, and many of those chemicals may have been detected. The following nine steps should be followed to organize the data into a form appropriate for a baseline risk assessment:

(1) gather all data available from the site investigation and sort by medium (Section 5.1);

(2) evaluate the analytical methods used (Section 5.2);

(3) evaluate the quality of data with respect to sample quantitation limits (Section 5.3);

(4) evaluate the quality of data with respect to qualifiers and codes (Section 5.4);

(5) evaluate the quality of data with respect to blanks (Section 5.5);

(6) evaluate tentatively identified compounds (Section 5.6);

(7) compare potential site-related contamination with background (Section 5.7);

(8) develop a set of data for use in the risk assessment (Section 5.8); and

(9) if appropriate, further limit the number of chemicals to be carried through the risk assessment (Section 5.9).

Prior to conducting any of these steps, the EPA remedial project manager (RPM) should be consulted to determine if certain steps should be modified, added, or deleted as a result of site-specific conditions. Also, some of the steps may be conducted outside the context of the risk assessment (e.g., for the feasibility study). The rationale for not evaluating certain data based on any of these steps must be fully discussed in the text of the risk assessment report.

The following sections address each of the data evaluation steps in detail, and Exhibit 5-1 presents a flowchart of the process. The outcome of this evaluation is (1) the identification of a set of chemicals that are likely to be site-related and (2) reported concentrations that are of acceptable quality for use in the quantitative risk assessment.

ACRONYMS FOR CHAPTER 5

CLP = Contract Laboratory Program
CRDL = Contract-Required Detection Limit
CRQL = Contract-Required Quantitation Limit
DL = Detection Limit
FIT = Field Investigation Team
IDL = Instrument Detection Limit
MDL = Method Detection Limit
ND = Non-detect
PE = Performance Evaluation
PQL = Practical Quantitation Limit
QA/QC = Quality Assurance/Quality Control
QL = Quantitation Limit
RAS = Routine Analytical Services
SAS = Special Analytical Services
SMO = Sample Management Office
SOW = Statement of Work
SQL = Sample Quantitation Limit
SVOC = Semivolatile Organic Chemical
TCL = Target Compound List
TIC = Tentatively Identified Compound
TOC = Total Organic Carbon
TOX = Total Organic Halogens
VOC = Volatile Organic Chemical

DEFINITIONS FOR CHAPTER 5

Chemicals of Potential Concern. Chemicals that are potentially site-related and whose data are of sufficient quality for use in the quantitative risk assessment.

Common Laboratory Contaminants. Certain organic chemicals (considered by EPA to be acetone, 2-butanone, methylene chloride, toluene, and the phthalate esters) that are commonly used in the laboratory and thus may be introduced into a sample from laboratory cross-contamination, not from the site.

Contract-required Quantitation Limit (CRQL). Chemical-specific levels that a CLP laboratory must be able to routinely and reliably detect and quantitate in specified sample matrices. May or may not be equal to the reported quantitation limit of a given chemical in a given sample.

Detection Limit (DL). The lowest amount that can be distinguished from the normal "noise" of an analytical instrument or method.

Non-detects (NDs). Chemicals that are not detected in a particular sample above a certain limit, usually the quantitation limit for the chemical in that sample. Non-detects may be indicated by a "U" data qualifier.

Positive Data. Analytical results for which measurable concentrations (i.e., above a quantitation limit) are reported. May have data qualifiers attached (except a U, which indicates a non-detect).

Quantitation Limit (QL). The lowest level at which a chemical can be accurately and reproducibly quantitated. Usually equal to the instrument detection limit multiplied by a factor of three to five, but varies for different chemicals and different samples.

If the nine data evaluation steps are followed, the number of chemicals to be considered in the remainder of the risk assessment usually will be less than the number of chemicals initially identified. Chemicals remaining in the quantitative risk assessment based upon this evaluation are referred to in this guidance as "chemicals of potential concern."

5.1 COMBINING DATA AVAILABLE FROM SITE INVESTIGATIONS

Gather data, which may be from several different sampling periods and based on several different analytical methods, from all available sources, including field investigation team (FIT) reports, remedial investigations, preliminary site assessments, and ongoing site characterization and alternatives screening activities. Sort data by medium. A useful table format for presenting data is shown in Exhibit 5-2.

Evaluate data from different time periods to determine if concentrations are similar or if changes have occurred between sampling periods. If the methods used to analyze samples from different time periods are similar in terms of the types of analyses conducted and the QA/QC procedures followed, and if the concentrations between sampling periods are similar, then the data may be combined for the purposes of quantitative risk assessment in order to obtain more information to characterize the site. If concentrations of chemicals change significantly between sampling periods, it may be useful to keep the data separate and evaluate risks separately. Alternatively, one could use only the most recent data in the quantitative risk assessment and evaluate older data in a qualitative analysis of changes in concentrations over time. The RPM should be consulted on the elimination of any data sets from the risk assessment, and justification for such elimination must be fully described in the risk assessment report.

EXHIBIT 5-1
DATA EVALUATION

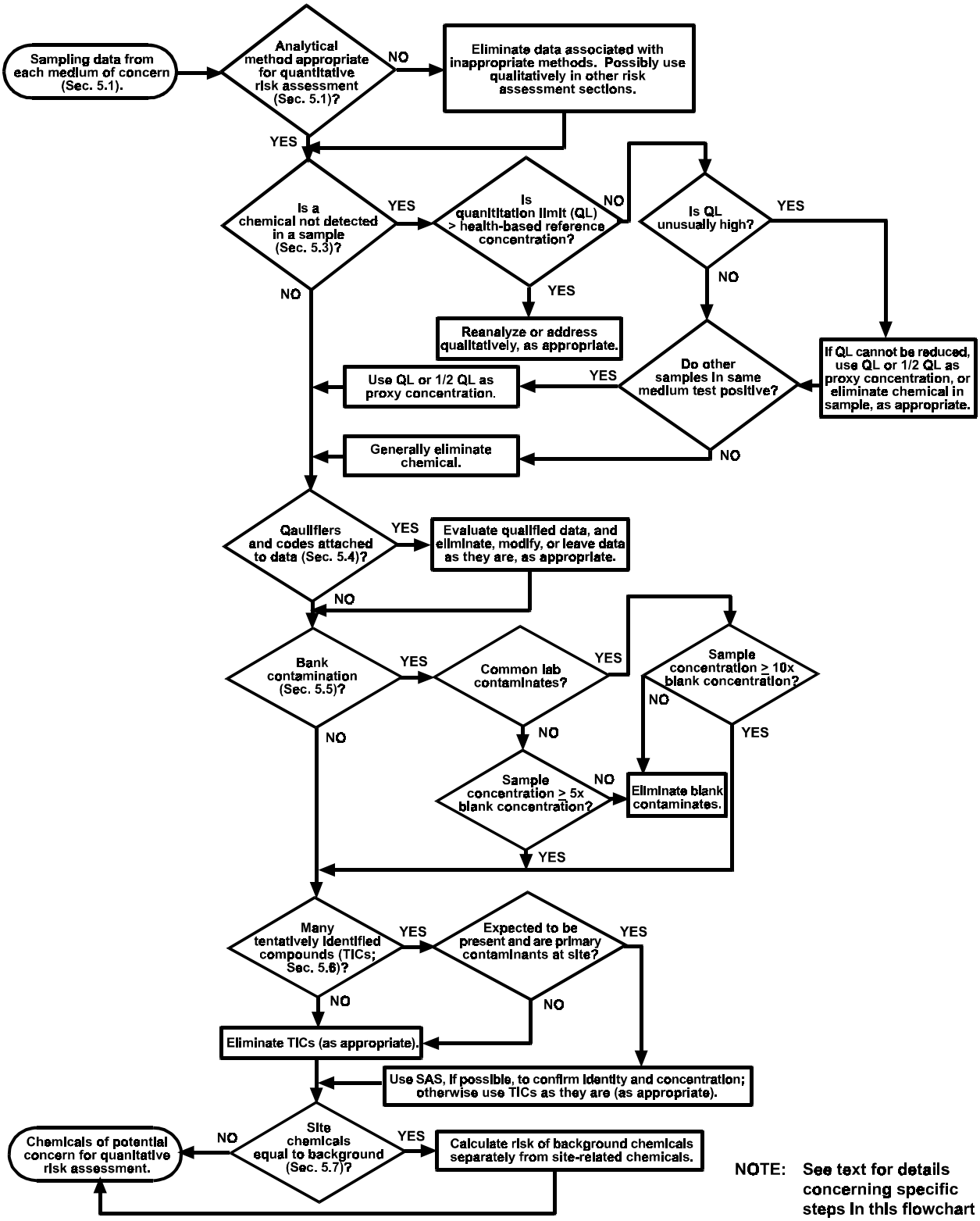


EXHIBIT 5-2

EXAMPLE OF OUTPUT FORMAT FOR VALIDATED DATA

	Area X		
Sample Medium	Soil	Soil	Soil
Sample ID	SRB-3-1	SRB-3-1DU	SRB-3-2
Sample or Screen Depth	0-1'	0-1'	2-4'
Date Collected	12/14/87	12/14/87	12/10/87
Units	ug/kg	ug/kg	ug/kg
Blanks or Duplicates		Duplicate	

Chemical	CRQL[a]	Concentration	Qualifier[b]	CRQL[a]	Concentration	Qualifier[b]	CRQL[a]	Concentration	Qualifier[b]
Aroclor-1016	80	80	U	80	80	U	2000[c]	2000	UJ
Aroclor-1221	80	80	U	80	80	U	2000[c]	2000	UJ
Aroclor-1232	80	80	U	80	80	U	2000[c]	2000	UJ
Aroclor-1242	80	40	J	80	42	J	2000[c]	2000	UJ
Aroclor-1248	80	30	J	80	36	J	2000[c]	2000	UJ
Aroclor-1254	160	120	J	160	110	J	2000[c]	1800	J
Aroclor-1260	160	210		160	220		2000[c]	2100	

Note: All values other than qualifiers must be entered as numbers, not as labels.

[a] Contract-required quantitation limit (unless otherwise noted). Values for illustration only.

[b] Refer to Section 5.4 for an explanation of qualifiers.

[c] Sample quantitation limit.

5.2 EVALUATION OF ANALYTICAL METHODS

Group data according to the types of analyses conducted (e.g., field screening analysis, semivolatiles analyzed by EPA methods for water and wastewater, semivolatiles analyzed by EPA's Superfund Contract Laboratory Program [CLP] procedures) to determine which analytical method results are appropriate for use in quantitative risk assessment. Often, this determination has been made already by regional and contractor staff.

An overview of EPA analytical methods is provided in the box below. Exhibit 5-3 presents examples of the types of data that are not usually appropriate for use in quantitative risk assessment, even though they may be available from a site investigation.

OVERVIEW OF THE CLP AND OTHER EPA ANALYTICAL METHODS

The EPA Contract Laboratory Program (CLP) is intended to provide analytical services for Superfund waste site samples. As discussed in the *User's Guide to the Contract Laboratory Program* (EPA 1988a, hereafter referred to as the CLP User's Guide), the program was developed to fill the need for legally defensible results supported by a high level of quality assurance (i.e., data of known quality) and documentation.

Prior to becoming CLP laboratories, analytical laboratories must meet stringent requirements for laboratory space and practices, instrumentation, personnel training, and quality control (QC), and also must successfully analyze performance evaluation (PE) samples. Before the first samples are shipped to the laboratory, audits of CLP labs are conducted to verify all representations made by laboratory management. Continuing performance is monitored by periodic PE sample analyses, routine and remedial audits, contract compliance screening of data packages, and oversight by EPA.

Superfund samples are most commonly analyzed using the Routine Analytical Services (RAS) conducted by CLP laboratories. Under RAS, all data are generated using the same analytical protocols specifying instrumentation, sample handling, analysis parameters, required quantitation limits, QC requirements, and report format. Protocols are provided in the *CLP Statement of Work (SOW) for Inorganics* (EPA 1988b) and the *CLP Statement of Work for Organics* (1988c). The SOWs also contain EPA's target analyte or compound lists (TAL for inorganics, TCL for organics), which are the lists of analytes and required quantitation limits (QLs) for which every Superfund site sample is routinely analyzed under RAS. As of June 1989, analytes on the TCL/TAL consist of 34 volatile organic chemicals (VOCs), 65 semivolatile organic chemicals (SVOCs), 19 pesticides, 7 polychlorinated biphenyls, 23 metals, and total cyanide. Finally, the SOW specifies data qualifiers that may be placed on certain data by the laboratory to communicate information and/or QC problems.

CLP labs are required to submit RAS data packages to EPA's Sample Management Office (SMO) and to the EPA region from which the samples originated within 35 days of receipt of samples. SMO provides management, operational, and administrative support to the CLP to facilitate optimal use of the program. SMO personnel identify incomplete or missing elements and verify compliance with QA/QC requirements in the appropriate SOW. In addition to the SMO review, all CLP data are inspected by EPA-appointed regional data validators. Using Laboratory Data Validation Functional Guidelines issued by EPA headquarters (hereafter referred to as Functional Guidelines for Inorganics [EPA 1988d] and Functional Guidelines for Organics [EPA 1988e]), regional guidelines, and professional judgment, the person validating data identifies deviations from the SOW, poor QC results, matrix interferences, and other analytical problems that may compromise the potential uses of the data. In the validation process, data may be flagged with qualifiers to alert data users of deviations from QC requirements. These qualifiers differ from those qualifiers attached to the data by the laboratory.

In addition to RAS, non-standard analyses may be conducted using Special Analytical Services (SAS) to meet user requirements such as short turnaround time, lower QLs, non-standard matrices, and the testing of analytes other than those on the Target Compound List. Under SAS, the user requests specific analyses, QC procedures, report formats, and timeframe needed.

Examples of other EPA analytical methods include those described in *Test Methods for Evaluating Solid Waste* (EPA 1986; hereafter referred to as SW-846 Methods) and *Methods for Organic Chemical Analysis of Municipal and Industrial Wastewater* (EPA 1984; hereafter referred to as EPA 600 Methods). The SW-846 Methods provide analytical procedures to test solid waste to determine if it is a hazardous waste as defined under the Resource Conservation and Recovery Act (RCRA). These methods include procedures for collecting solid waste samples and for determining reactivity, corrosivity, ignitability, composition of waste, and mobility of waste components. The EPA 600 Methods are used in regulatory programs under the Clean Water Act to determine chemicals present in municipal and industrial wastewaters.

EXHIBIT 5-3

EXAMPLES OF THE TYPES OF DATA POTENTIALLY UNSUITABLE FOR A QUANTITATIVE RISK ASSESSMENT

Analytical Instrument or Method	Purpose of Analysis	Analytical Result
HNu Organic Vapor Detector	Health and Safety, Field Screen	Total Organic Vapor
Organic Vapor Analyzer	Health and Safety, Field Screen	Total Organic Vapor
Combustible Gas Indicator	Health and Safety	Combustible Vapors, Oxygen-deficient Atmosphere
Field Gas Chromatography[a]	Field Screen/Analytical Method	Specific Volatile and Semi-volatile Organic Chemicals

[a] Depending on the detector used, this instrument can be sufficiently sensitive to yield adequate data for use in quantitative risk assessment; however, a confirming analysis by GC/MS should be performed on a subset of the samples in a laboratory prior to use.

Analytical results that are not specific for a particular compound (e.g., total organic carbon [TOC], total organic halogens [TOX]) or results of insensitive analytical methods (e.g., analyses using portable field instruments such as organic vapor analyzers and other field screening methods) may be useful when considering sources of contamination or potential fate and transport of contaminants. These types of analytical results, however, generally are not appropriate for quantitative risk assessment; therefore, the risk assessor may not want to include them in the summary of chemicals of potential concern for the quantitative risk assessment. In addition, the results of analytical methods associated with unknown, few, or no QA/QC procedures should be eliminated from further quantitative use. These types of results, however, may be useful for qualitative discussions of risk in other sections of the risk assessment report.

The outcome of this step is a set of site data that has been developed according to a standard set of sensitive, chemical-specific methods (e.g., SW-846 Methods [EPA 1986], EPA 600 Methods [EPA 1984], CLP Statements of Work [EPA 1988b,c]), with QA/QC procedures that are well-documented and traceable. The data resulting from analyses conducted under the CLP, which generally comprise the majority of results available from a Superfund site investigation, fall into this category.

Although the CLP was developed to ensure that consistent QA/QC methods are used when analyzing Superfund site samples, it does not ensure that all analytical results are consistently of sufficient quality and reliability for use in quantitative risk assessment. Neither the CLP nor QA/QC procedures associated with other methods make judgments concerning the ultimate "usability" of the data. Do not accept at face value all remaining analytical results, whether from the CLP or from some other set of analytical methodologies. Instead, determine -- according to the steps discussed below -- the limitations and uncertainties associated with the data so that only data that are appropriate and reliable for use in a quantitative risk assessment are carried through the process.

5.3 EVALUATION OF QUANTITATION LIMITS

This step involves evaluation of quantitation limits and detection limits (QLs and DLs) for all of the chemicals assessed at the site. This evaluation may lead to the re-analysis of some samples, the use of "proxy" (or estimated) concentrations, and/or the elimination of certain chemicals from further consideration (because they are believed to be absent from the site). Types and definitions of QLs and DLs are presented in the box on the next page.

Before eliminating chemicals because they are not detected (or conducting any other manipulation of the data), the following points should be considered:

(1) the sample quantitation limit (SQL) of a chemical may be greater than corresponding standards, criteria, or concentrations derived from toxicity reference values (and, therefore, the chemical may be present at levels greater than these corresponding reference concentrations, which may result in undetected risk); and

(2) a particular SQL may be significantly higher than positively detected values in other samples in a data set.

These two points are discussed in detail in the following two subsections. A third subsection provides guidance for situations where only some of the samples for a given medium test positive for a particular chemical. A fourth subsection addresses the special situation where SQLs are not available. The final subsection addresses the specific steps involved with elimination of chemicals from the quantitative risk assessment based on their QLs.

5.3.1 SAMPLE QUANTITATION LIMITS (SQLs) THAT ARE GREATER THAN REFERENCE CONCENTRATIONS

As discussed in Chapter 4, QLs needed for the site investigation should be specified in the sampling plan. For some chemicals, however,

SQLs obtained under RAS or SAS may exceed certain reference concentrations (e.g., maximum contaminant levels [MCLs], concentrations corresponding to a 10^{-6} cancer risk). The box on the next page illustrates this problem. For certain chemicals (e.g., antimony), the CLP contract-required quantitation limits (CRQLs) exceed the corresponding reference concentrations for noncarcinogenic effects, based on the EPA-verified reference dose and a 2-liter per day ingestion of water by a 70-kilogram person.[1] Estimation of cancer risks for several other chemicals (e.g., arsenic, styrene) at their CRQLs yields cancer risks exceeding 10^{-4}, based on the same water ingestion factors. Most potential carcinogens with EPA-derived slope factors have CRQLs that yield cancer risk levels exceeding 10^{-6} in water, and none of the carcinogens with EPA-derived slope factors have CRQL values yielding less than 10^{-7} cancer risk levels (as of the publication date of this manual; data not shown).

Three points should be noted when considering this example.

(1) Review of site information and a preliminary determination of chemicals of potential concern at a site prior to sample collection may allow the specification of lower QLs (i.e., using SAS) before an investigation begins (see Chapter 4). This is the most efficient way to minimize the problem of QLs exceeding levels of potential concern.

(2) EPA's Analytical Operations Branch currently is working to reduce the CRQL values for several chemicals on the TCL and TAL, and to develop an analytical service for chemicals with special standards (e.g., MCLs).

TYPES AND DEFINITIONS OF DETECTION LIMITS AND QUANTITATION LIMITS

Strictly interpreted, the detection limit (DL) is the lowest amount of a chemical that can be "seen" above the normal, random noise of an analytical instrument or method. A chemical present below that level cannot reliably be distinguished from noise. DLs are chemical-specific and instrument-specific and are determined by statistical treatment of multiple analyses in which the ratio of the lowest amount observed to the electronic noise level (i.e., the signal-to-noise ratio) is determined. On any given day in any given sample, the calculated limit may not be attainable; however, a properly calculated limit can be used as an overall general measure of laboratory performance.

Two types of DLs may be described -- instrument DLs (IDLs) and method DLs (MDLs). The IDL is generally the lowest amount of a substance that can be detected by an instrument; it is a measure only of the DL for the instrument, and does not consider any effects that sample matrix, handling, and preparation may have. The MDL, on the other hand, takes into account the reagents, sample matrix, and preparation steps applied to a sample in specific analytical methods.

Due to the irregular nature of instrument or method noise, reproducible quantitation of a chemical is not possible at the DL. Generally, a factor of three to five is applied to the DL to obtain a quantitation limit (QL), which is considered to be the lowest level at which a chemical may be accurately and reproducibly quantitated. DLs indicate the level at which a small amount would be "seen," whereas QLs indicate the levels at which measurements can be "trusted."

Two types of QLs may be described -- contract-required QLs (CRQLs) and sample QLs (SQLs). (Contract-required detection limits [CRDL] is the term used for inorganic chemicals. For the purposes of this manual, however, CRQL will refer to both organic and inorganic chemicals.) In order to participate in the CLP, a laboratory must be able to meet EPA CRQLs. CRQLs are chemical-specific and vary depending on the medium analyzed and the amount of chemical expected to be present in the sample. As the name implies, CRQLs are not necessarily the lowest detectable levels achievable, but rather are levels that a CLP laboratory should routinely and reliably detect and quantitate in a variety of sample matrices. A specific sample may require adjustments to the preparation or analytical method (e.g., dilution, use of a smaller sample aliquot) in order to be analyzed. In these cases, the reported QL must in turn be adjusted. Therefore, SQLs, not CRQLs, will be the QLs of interest for most samples. In fact, for the same chemical, a specific SQL may be higher than, lower than, or equal to SQL values for other samples. In addition, preparation or analytical adjustments such as dilution of a sample for quantitation of an extremely high level of only one compound could result in non-detects for all other compounds included as analytes for a particular method, even though these compounds may have been present at trace quantities in the undiluted sample. Because SQLs take into account sample characteristics, sample preparation, and analytical adjustments, these values are the most relevant QLs for evaluating non-detected chemicals.

EXAMPLE OF HEALTH RISKS FROM INGESTION OF WATER CONTAMINATED WITH SELECTED CHEMICALS AT THEIR QUANTITATION LIMITS[a]

Chemical	CAS #	CRQL or CRDL (ug/L)[b]	Cancer Risk CRDL/RfC[c]	at CRQL or CRDL[d]
Antimony	7440-36-0	60	4.3	
Arsenic	7440-38-2	10	$5x10^{-4}$	
Benz(a)pyrene	50-32-8	10		$3x10^{-3}$
Bis(2-Chloroethyl)ether	111-44-4	10		$3x10^{-4}$
2,4-Dinitrotoluene	121-14-2	10		$2x10^{-4}$
Hexachlorobenzene	118-74-1	10		$5x10^{-4}$
N-Nitroso-di-n-dipropylamine	621-64-7	10		$2x10^{-3}$
PCB-1254	11096-69-1	1	$2x10^{-4}$[e]	
PCB-1260	11096-82-5	1	$2x10^{-4}$	
Styrene	100-42-5	5	$4x10^{-4}$	
Vinyl chloride	75-01-4	10		$7x10^{-4}$

[a] All values in this example are for illustration purposes only.

[b] CRQL = Contract-required quantitation limit (organics) of the Contract Laboratory Program (revised April 1989).
CRDL = Contract-required detection limit (inorganics) of the Contract Laboratory Program (revised July 1988).

The CRQL and CRDL values presented here are for the regular multi-media multi-concentration CLP methods.

[c] RfC = Reference concentration (based on the August 1989 reference dose for oral exposure, assuming a 70-kilogram adult drinks 2 liters of contaminated water per day).

[d] Cancer Risk at CRQL or CRDL = Excess upper-bound lifetime cancer risk (based on the August 1989 slope factor for oral exposure, assuming a 70-kilogram adult drinks 2 liters of contaminated water per day).

[e] PCB-1260 slope factor was used.

(3) In several situations, an analytical laboratory may be able to attain QLs in particular samples that are below or above the CRQL values.

If SAS was not specified before sampling began and/or if a chemical is not detected in any sample from a particular medium at the QL, then available modeling data, as well as professional judgment, should be used to evaluate whether the chemical may be present above reference concentrations. If the available information indicates the chemical is not present, see Section 5.3.5 for guidance on eliminating chemicals. If there is some indication that the chemical is present, then either re-analyze selected samples using SAS, if time allows, or address the chemical qualitatively. In determining which option is most appropriate for a site, a screening-level risk assessment should be performed by assuming that the chemical is present in the sample at the SQL (see Section 5.3.4 for situations where SQLs are not available). Carry the chemical through the screening risk assessment, essentially conducting the assessment on the SQL for the particular chemical. In this way, the risks that would be posed if the chemical is present at the SQL can be compared with risks posed by other chemicals at the site.

Re-analyze the sample. This (preferred) option discourages elimination of questionable chemicals (i.e., chemicals that may be present below their QL but above a level of potential concern) from the risk assessment. If time allows and a sufficient quantity of the sample is available, submit a SAS request to re-analyze the sample at QLs that are below reference concentrations. The possible outcome of

this option is inclusion of chemicals positively detected at levels above reference concentrations but below the QLs that would normally have been attained under routine analysis of Superfund samples in the CLP program.

Address the chemical qualitatively. A second and less desirable option for a chemical that may be present below its QL (and possibly above its health-based reference concentration) is to eliminate the chemical from the quantitative risk assessment, noting that if the chemical was detected at a lower QL, then its presence and concentration could contribute significantly to the estimated risks.

5.3.2 UNUSUALLY HIGH SQLs

Due to one or more sample-specific problems (e.g., matrix interferences), SQLs for a particular chemical in some samples may be unusually high, sometimes greatly exceeding the positive results reported for the same chemical in other samples from the data set. Even if these SQLs do not exceed health-based standards or criteria, they may still present problems. If the SQLs cannot be reduced by re-analyzing the sample (e.g., through the use of SAS or sample cleaning procedures to remove matrix interferences), exclude the samples from the quantitative risk assessment if they cause the calculated exposure concentration (i.e., the concentration calculated according to guidance in Chapter 6) to exceed the maximum detected concentration for a particular sample set. The box on this page presents an example of how to address a situation with unusually high QLs.

EXAMPLE OF UNUSUALLY HIGH QUANTIFICATION LIMITS

In this example, concentrations of semivolatile organic chemicals in soils have been determined using the CLP's RAS.

	Concentration (ug/kg)			
Chemical	Sample 1	Sample 2	Sample 3	Sample 4
Phenol	330 U[a]	390	19,000 U	490

[a] U = Compound was analyzed for, but not detected. Value presented (e.g., 330 U) is the SQL.

The QLs presented in this example (i.e., 330 to 19,000 ug/kg) vary widely from sample to sample. SAS would not aid in reducing the unusually high QL of 19,000 ug/kg noted in Sample 3, assuming it was due to unavoidable matrix interferences. In this case, the result for phenol in Sample 3 would be eliminated from the quantitative risk assessment because it would cause the calculated exposure concentrations (from Chapter 6) to exceed the maximum detected concentration (in this case 490 ug/kg). Thus, the data set would be reduced to three samples: the non-detect in Sample 1 and the two detected values in Samples 2 and 4.

5.3.3 WHEN ONLY SOME SAMPLES IN A MEDIUM TEST POSITIVE FOR A CHEMICAL

Most analytes at a site are not positively detected in <u>each</u> sample collected and analyzed. Instead, for a particular chemical the data set generally will contain some samples with positive results and others with non-detected results. The non-detected results usually are reported as SQLs. These limits indicate that the chemical was not measured above certain levels, which may vary from sample to sample. The chemical may be present at a concentration just <u>below</u> the reported quantitation limit, or it may not be present in the sample at all (i.e., the concentration in the sample is zero).

In determining the concentrations most representative of potential exposures at the site (see Chapter 6), consider the positively detected results together with the non-detected results (i.e., the SQLs). If there is reason to believe that the chemical is present in a sample at a concentration below the SQL, use one-half of the SQL as a proxy concentration. The SQL value itself can be used if there is reason to believe the concentration is closer to it than to one-half the SQL. (See the next subsection for situations where SQLs are not available.) Unless site-specific information indicates that a chemical is not likely to be present in a sample, do not substitute the value zero in place of the SQL (i.e., do not assume that a chemical that is not detected at the SQL would not be detected in the sample if the analysis was extremely sensitive). Also, do not simply omit the non-detected results from the risk assessment.

5.3.4 WHEN SQLs ARE NOT AVAILABLE

A fourth situation concerning QLs may sometimes be encountered when evaluating site data. For some sites, data summaries may not provide the SQLs. Instead, MDLs, CRQLs, or even IDLs may have been substituted wherever a chemical was not detected. Sometimes, no detection or quantitation limits may be provided with the data. As a first step in these situations, always attempt to obtain the SQLs, because these are the most appropriate limits to consider when evaluating non-detected chemicals (i.e., they account for sample characteristics, sample preparation, or analytical adjustments that may differ from sample to sample).

If SQLs cannot be obtained, then, for CLP sample analyses, the CRQL should be used as the QL of interest for each non-detected chemical, with the understanding that these limits may overestimate or underestimate the actual SQL. For samples analyzed by methods different from CLP methods, the MDL may be used as the QL, with the understanding that in most cases this will underestimate the SQL (because the MDL is a measure of detection limits only and does not account for sample characteristics or matrix interferences). Note that the IDL should rarely be used for non-detected chemicals since it is a measure only of the detection limit for a particular instrument and does not consider the effect of sample handling and preparation or sample characteristics.

5.3.5 WHEN CHEMICALS ARE NOT DETECTED IN ANY SAMPLES IN A MEDIUM

After considering the discussion provided in the above subsections, generally eliminate those chemicals that have not been detected in any samples of a particular medium. On CLP data reports, these chemicals will be designated in each sample with a U qualifier preceded by the SQL or CRQL (e.g., 10 U). If information exists to indicate that the chemicals are present, they should not be eliminated. For example, if chemicals with similar transport and fate characteristics are detected frequently in soil at a site, and some of these chemicals also are detected frequently in ground water while the others are not detected, then the undetected chemicals are probably present in the ground water and therefore may need to be included in the risk assessment as ground-water contaminants.

The outcome of this step is a data set that only contains chemicals for which positive data (i.e., analytical results for which measurable concentrations are reported) are available in at least one sample from each medium. Unless otherwise indicated, assume at this point in the evaluation of data that positive data to which no uncertainties are attached concerning either the assigned identity of the chemical or the reported concentration (i.e., data that are not "tentative," "uncertain," or "qualitative") are appropriate for use in the quantitative risk assessment.

5.4 EVALUATION OF QUALIFIED AND CODED DATA

For CLP analytical results, various qualifiers and codes (hereafter referred to as qualifiers) are attached to certain data by either the laboratories conducting the analyses or by persons performing data validation. These qualifiers often pertain to QA/QC problems and generally indicate questions concerning chemical identity, chemical concentration, or both. All qualifiers must be addressed before the chemical can be used in quantitative risk assessment. Qualifiers used by the laboratory may differ from those used by data validation personnel in either identity or meaning.

5.4.1 TYPES OF QUALIFIERS

A list of the qualifiers that laboratories are permitted to use under the CLP -- and their potential use in risk assessment -- is presented in Exhibit 5-4. A similar list addressing data validation qualifiers is provided in Exhibit 5-5. In general, because the data validation process is intended to assess the effect of QC issues on data usability, validation data qualifiers are attached to the data after the laboratory qualifiers and supersede the laboratory qualifiers. If data have both laboratory and validation qualifiers and they appear contradictory, ignore the laboratory qualifier and consider only the validation qualifier. If qualifiers have been attached to certain data by the laboratory and have not been removed, revised, or superseded during data validation, then evaluate the

EXHIBIT 5-4

CLP LABORATORY DATA QUALIFIERS AND THEIR POTENTIAL USE IN QUANTITATIVE RISK ASSESSMENT

Qualifier	Definition	Indicates: Uncertain Identity?	Uncertain Concentration?	Include Data in Quantitative Risk Assessment?
Inorganic Chemical Data:[a]				
B	Reported value is <CRDL, but >IDL.	No	No	Yes
U	Compound was analyzed for, but not detected.	Yes	Yes	?
E	Value is estimated due to matrix interferences.	No	Yes	Yes
M	Duplicate injection precision criteria not met.	No	Yes	Yes
N	Spiked sample recovery not within control limits.	No	Yes	Yes
S	Reported value was determined by the Method of Standard Additions (MSA).	No	No	Yes
W	Post-digestion spike for furnace AA analysis is out of control limits, while sample absorbance is <50% of spike absorbance.	No	Yes	Yes
*	Duplicate analysis was not within control limits.	No	Yes	Yes
+	Correlation coefficient for MSA was <0.995.	No	Yes	Yes
Organic Chemical Data:[b]				
U	Compound was analyzed for, but not detected.	Yes	Yes	?but not

(continued)

EXHIBIT 5-4 (continued)

CLP LABORATORY DATA QUALIFIERS AND THEIR POTENTIAL USE IN QUANTITATIVE RISK ASSESSMENT

Qualifier	Definition	Indicates: Uncertain Identity?	Uncertain Concentration?	Include Data in Quantitative Risk Assessment?
J	Value is estimated, either for a tentatively identified compound (TIC) or when a compound is present (spectral identification criteria are met, but the value is <CRQL).	No, for TCL chemicals; Yes, for TICs	Yes	?
C	Pesticide results were confirmed by GC/MS.	No	No	Yes
B	Analyte found in associated blank as well as in sample.[c]	No	Yes	Yes
E	Concentration exceeds calibration range of GC/MS instrument.	No	Yes	Yes
D	Compound identified in an analysis at a secondary dilution factor.	No	No	Yes
A	The TIC is a suspected aldol-condensation product.	Yes	Yes	No
X	Additional flags defined separately.	--	--	--

-- = Data will vary with laboratory conducting analyses.

[a] Source: EPA 1988b.

[b] Source: EPA 1988c.[c] See Section 5.5 for guidance concerning blank contamination.

EXHIBIT 5-5

VALIDATION DATA QUALIFIERS AND THEIR POTENTIAL USE IN QUANTITATIVE RISK ASSESSMENT

Qualifier	Definition	Indicates: Uncertain Identity?	Uncertain Concentration?	Include Data in Quantitative Risk Assessment?
Inorganic and Organic Chemical Data:[a]				
U	The material was analyzed for, but not detected. The associated numerical value is the SQL.	Yes	Yes	?
J	The associated numerical value is an estimated quantity.	No	Yes	Yes
R	Quality control indicates that the data are unusable (compound may or may not be present). Re-sampling and/or re-analysis is necessary for verification.	Yes	Yes	No
Z	No analytical result (inorganic data only).	--	--	--
Q	No analytical result (organic data only).	--	--	--
N	Presumptive evidence of presence of material (tentative identification).[b]	Yes	Yes	?

-- = Not applicable

[a] Source: EPA 1988d,e.

[b] Organic chemical data only.

laboratory qualifier itself. If it is unclear whether the data have been validated, contact the appropriate data validation and/or laboratory personnel.

The type of qualifier and other site-specific factors determine how qualified data are to be used in a risk assessment. As seen in Exhibits 5-4 and 5-5, the type of qualifier attached to certain data often indicates how that data should be used in a risk assessment. For example, most of the laboratory qualifiers for both inorganic chemical data and organic chemical data (e.g., J, E, N) indicate uncertainty in the reported concentration of the chemical, but not in its assigned identity. Therefore, these data can be used just as positive data with no qualifiers or codes. In general, include data with qualifiers that indicate uncertainties in concentrations but not in identification.

Examples showing the use of certain qualified data are presented in the next two boxes. The first box addresses the J qualifier, the most commonly encountered data qualifier in Superfund data packages. Basically, the guidance here is to use J-qualified concentrations the same way as positive data that do not have this qualifier. If possible, note potential uncertainties associated with the qualifier, so that if data qualified with a J contribute significantly to the risk, then appropriate caveats can be attached.

EXAMPLE OF J QUALIFIERS

In this example, concentrations of volatile organic chemicals in ground water have been determined using the CLP's RAS.

	Concentration (ug/L)			
Chemical	Sample 1	Sample 2	Sample 3	Sample 4
Tetrachloro-ethene	14,000 J[a]	40	30 U[b]	20 J

[a] J = The numerical value is an estimated quantity.
[b] U = Compound was analyzed for, but not detected. Value presented (e.g., 30 U) is the SQL.

Tetrachlorethene was detected in three of four samples at concentrations of 14,000 µg/1, 40 µg/1, and 20 ug/1; therefore, these concentrations -- as well as the non-detect -- should be used in determining representative concentrations.

An illustration of the use of R-qualified data is presented in the box in this column. The definition, and therefore the use of the R qualifier, differs depending on whether the data have been validated or not. (Note that the CLP formerly used R as a laboratory qualifier to indicate low spike recovery for inorganics. This has been changed, but older data may still have been qualified by the laboratory with an R.) If it is known that the R data qualifier indicates that the sample result was rejected by the data validation personnel, then this result should be eliminated from the risk assessment; if the R data qualifier was placed on the data to indicate estimated data due to low spike recovery (i.e., the R was placed on the data by the laboratory and not by the validator), then use the R-qualified data in a manner similar to the use of J-qualified data (i.e., use the R-qualified concentrations the same way as positive data that do not have this qualifier). If possible, note whether the R-qualified data are overestimates or underestimates of actual expected chemical concentrations so that appropriate caveats may be attached if data qualified with an R contribute significantly to the risk.

EXAMPLE OF VALIDATED DATA CONTAINING R QUALIFIERS

In this example, concentrations of inorganic chemicals in ground water have been determined using the CLP's RAS.

	Concentration (ug/L)			
Chemical	Sample 1	Sample 2	Sample 3	Sample 4
Manganese	310	500 R[a]	30 UR[b]	500

[a] R = Quality control indicates that the data are unusable (compound may or may not be present).

[b] U = Compound was analyzed for, but not detected. Value presented (e.g., 30 U) is the SQL.

These data have been validated, and therefore the R qualifiers indicate that the person conducting the data validation rejected the data for manganese in Samples 2 and 3. The "UR" qualifier means that manganese was not detected in Sample 3; however, the data validator rejected the non-detected result. Eliminate these two samples so that the data set now consists of only two samples (Samples 1

5.4.2 USING THE APPROPRIATE QUALIFIERS

The information presented in Exhibits 5-4 and 5-5 is based on the most recent EPA guidance documents concerning qualifiers: the SOW for Inorganics and the SOW for Organics (EPA 1988b,c) for laboratory qualifiers, and the Functional Guidelines for Inorganics and the Functional Guidelines for Organics (EPA 1988d,e) for validation qualifiers. The types and definitions of qualifiers, however, may be periodically updated within the CLP program. In addition, certain EPA regions may have their own data qualifiers and associated definitions. These regional qualifiers are generally consistent with the Functional Guidelines, but are designed to convey additional information to data users.

In general, the risk assessor should check whether the information presented in this section is current by contacting the appropriate regional CLP or headquarters Analytical Operations Branch staff. Also, if definitions are not reported with the data, regional contacts should be consulted prior to evaluating qualified data. These variations may affect how data with certain qualifiers should be used in a risk assessment. Make sure that definitions of data qualifiers used in the data set for the site have been reported with the data and are current. Never guess about the definition of qualifiers.

5.5 COMPARISON OF CONCENTRATIONS DETECTED IN BLANKS WITH CONCENTRATIONS DETECTED IN SAMPLES

Blank samples provide a measure of contamination that has been introduced into a sample set either (1) in the field while the samples were being collected or transported to the laboratory or (2) in the laboratory during sample preparation or analysis. To prevent the inclusion of non-site-related contaminants in the risk assessment, the concentrations of chemicals detected in blanks must be compared with concentrations of the same chemicals detected in site samples. Detailed definitions of different types of blanks are provided in the box on the next page.

Blank data should be compared with results from samples with which the blanks are associated. It is often impossible, however, to determine the association between certain blanks and data. In this case, compare the blank data with results from the entire sample data set. Use the guidelines in the following paragraphs when comparing sample concentrations with blank concentrations.

Blanks containing common laboratory contaminants. As discussed in the CLP SOW for Organics (EPA 1988c) and the Functional Guidelines for Organics (EPA 1988e), acetone, 2-butanone (or methyl ethyl ketone), methylene chloride, toluene, and the phthalate esters are considered by EPA to be common laboratory contaminants. In accordance with the Functional Guidelines for Organics (EPA 1988e) and the Functional Guidelines for Inorganics (EPA 1988d), if the blank contains detectable levels of common laboratory contaminants, then the sample results should be considered as positive results only if the concentrations in the sample exceed ten times the maximum amount detected in any blank. If the concentration of a common laboratory contaminant is less than ten times the blank concentration, then conclude that the chemical was not detected in the particular sample and, in accordance with EPA guidance, consider the blank-related concentrations of the chemical to be the quantitation limit for the chemical in that sample. Note that if all samples contain levels of a common laboratory contaminant that are less than ten times the level of contamination noted in the blank, then completely eliminate that chemical from the set of sample results.

TYPES OF BLANKS

Blanks are analytical quality control samples analyzed in the same manner as site samples. They are used in the measurement of contamination that has been introduced into a sample either (1) in the field while the samples were being collected or transported to the laboratory or (2) in the laboratory during sample preparation or analysis. Four types of blanks -- trip, field, laboratory calibration, and laboratory reagent (or method) -- are described below. A discussion on the water used for the blank also is provided.

Trip Blank. This type of blank is used to indicate potential contamination due to migration of volatile organic chemicals (VOCs) from the air on the site or in sample shipping containers, through the septum or around the lid of sampling vials, and into the sample. A trip blank consists of laboratory distilled, deionized water in a 40-ml glass vial sealed with a teflon septum. The blank accompanies the empty sample bottles to the field as well as the samples returning to the laboratory for analysis; it is not opened until it is analyzed in the lab with the actual site samples. The containers and labels for trip blanks should be the same as the containers and labels for actual samples, thus making the laboratory "blind" to the identity of the blanks.

Field Blank. A field blank is used to determine if certain field sampling or cleaning procedures (e.g., insufficient cleaning of sampling equipment) result in cross-contamination of site samples. Like the trip blank, the field blank is a sample of distilled, deionized water taken to the field with empty sample bottles and is analyzed in the laboratory along with the actual samples. Unlike the trip blank, however, the field blank sample is opened in the field and used as a sample would be (e.g., it is poured through cleaned sampling equipment or it is poured from container to container in the vicinity of a gas-powered pump). As with trip blanks, the field blanks' containers and labels should be the same as for actual samples.

Laboratory Calibration Blank. This type of blank is distilled, deionized water injected directly into an instrument without having been treated with reagents appropriate to the analytical method used to analyze actual site samples. This type of blank is used to indicate contamination in the instrument itself, or possibly in the distilled, deionized water.

Laboratory Reagent or Method Blank. This blank results from the treatment of distilled, deionized water with all of the reagents and manipulations (e.g., digestions or extractions) to which site samples will be subjected. Positive results in the reagent blank may indicate either contamination of the chemical reagents or the glassware and implements used to store or prepare the sample and resulting solutions. Although a laboratory following good laboratory practices will have its analytical processes under control, in some instances method blank contamination cannot be entirely eliminated.

Water Used for Blanks. For all the blanks described above, results are reliable only if the water comprising the blank was clean. For example, if the laboratory water comprising the trip blank was contaminated with VOCs prior to being taken to the field, then the source of VOC contamination in the trip blank cannot be isolated (see laboratory calibration blank).

Blanks containing chemicals that are not common laboratory contaminants. As discussed in the previously referenced guidance, if the blank contains detectable levels of one or more organic or inorganic chemicals that are not considered by EPA to be common laboratory contaminants (e.g., all other chemicals on the TCL), then consider site sample results as positive only if the concentration of the chemical in the site sample exceeds five times the maximum amount detected in any blank. Treat samples containing less than five times the amount in any blank as non-detects and, in accordance with EPA guidance, consider the blank-related chemical concentration to be the quantitation limit for the chemical in that sample. Again, note that if all samples contain levels of a TCL chemical that are less than five times the level of contamination noted in the blank, then completely eliminate that chemical from the set of sample results.

5.6 EVALUATION OF TENTATIVELY IDENTIFIED COMPOUNDS

Both the identity and reported concentration of a tentatively identified compound (TIC) is questionable (see the box on the next page for background on TICs). Two options for addressing TICs exist, depending on the relative number of TICs compared to non-TICs.

5.6.1 WHEN FEW TICs ARE PRESENT

When only a few TICs are present compared to the TAL and TCL chemicals, and no historical or other site information indicates that either a particular TIC may indeed be present at the site (e.g., because it may be a by-product of a chemical operation conducted when the site was active) or that the estimated concentration may be very high (i.e., the risk would be dominated by the TIC), then generally do not include the TICs in the risk assessment. Otherwise, follow the guidance provided in the next subsection. Consult with the RPM about omitting TICs from the quantitative risk assessment, and document reasons for excluding TICs in the risk assessment report.

TENTATIVELY IDENTIFIED COMPOUNDS

EPA's TCL may be a limited subset of the organic compounds that could actually be encountered at a particular site. Thus, although the CLP RAS requires the laboratory to analyze samples only for compounds on the TCL, the analysis of VOCs and SVOCs may indicate the presence of additional organic compounds not on the TCL. These additional compounds are shown by "peaks" on the chromatograms. (A chromatogram is a paper representation of the response of the instrument to the presence of a compound.) The CLP laboratory must attempt to identify the 30 highest peaks (10 VOCs and 20 SVOCs) using computerized searches of a library containing mass spectra (essentially "fingerprints" for particular compounds). When the mass spectra match to a certain degree, the compound (or general class of compound) is named; however, the assigned identity is in most cases highly uncertain. These compounds are called tentatively identified compounds (TICs).

The CLP SOW provides procedures to obtain a rough estimate of concentration of TICs. These estimates, however, are highly uncertain and could be orders of magnitude higher or lower than the actual concentration. For TICs, therefore, assigned identities may be inaccurate, and quantitation is certainly inaccurate. Due to these uncertainties, TIC information often is not provided with data summaries from site investigations. Additional sampling and analysis under SAS may reduce the uncertainty associated with TICs and, therefore, TIC information should be sought when it is absent from data summaries.

5.6.2 WHEN MANY TICs ARE PRESENT

If many TICs are present relative to the TAL and TCL compounds identified, or if TIC concentrations appear high or site information indicates that TICs are indeed present, then further evaluation of TICs is necessary. If sufficient time is available, use SAS to confirm the identity and to positively and reliably measure the concentrations of TICs prior to their use in the risk assessment. If SAS methods to identify and measure TICs are unavailable, or if there is insufficient time to use SAS, then the TICs should be included as chemicals of potential concern in the risk assessment and the uncertainty in both identity and concentration should be noted (unless information exists to indicate that the TICs are not present).

5.7 COMPARISON OF SAMPLES WITH BACKGROUND

In some cases, a comparison of sample concentrations with background concentrations (e.g., using the geometric mean concentrations of the two data sets) is useful for identifying the non-site-related chemicals that are found at or near the site. If background risk might be a concern, it should be calculated separately from site-related risk. Often, however, the comparison of samples with background is unnecessary because of the low risk usually posed by the background chemicals compared to site-related chemicals.

As discussed in Chapter 4, information collected during the RI can provide information on two types of background chemicals: (1) naturally occurring chemicals that have not been influenced by humans and (2) chemicals that are present due to anthropogenic sources. Either type of background chemical can be either localized or ubiquitous.

Information on background chemicals may have been obtained by the collection of site-specific background samples and/or from other sources (e.g., County Soil Conservation Service surveys, United States Geological Survey [USGS] reports). As discussed in Chapter 4, background

concentrations should be from the site or the vicinity of the site.

5.7.1 USE APPROPRIATE BACKGROUND DATA

Background samples collected during the site investigation should not be used if they were obtained from areas influenced or potentially influenced by the site. Instead, the literature sources mentioned in the previous paragraph may be consulted to determine background levels of chemicals in the vicinity of the site. Care must be taken in using literature sources, because the data contained therein might represent nationwide variation in a particular parameter rather than variation typical of the geographic region or geological setting in which the site is located. For example, a literature source providing concentrations of chemicals in ground water on a national scale may show a wide range of concentrations that is not representative of the variation in concentrations that would be expected at a particular site.

5.7.2 IDENTIFY STATISTICAL METHODS

In cases where background comparisons will be made, any statistical methods that will be used should be identified prior to the collection of samples (see Chapter 4). Guidance documents and reports that are available to aid in background comparison are listed in Section 4.4.3. Prior to conducting the steps discussed in the next two subsections, the RPM should be consulted to determine the type of comparison to be made, if any. Both a justification for eliminating chemicals based on a background comparison and a brief overview of the type of comparison conducted should be included in the risk assessment report.

5.7.3 COMPARE CHEMICAL CONCENTRATIONS WITH NATURALLY OCCURRING LEVELS

As defined previously, naturally occurring levels are levels of chemicals that are present under ambient conditions and that have not been increased by anthropogenic sources. If inorganic chemicals are present at the site at naturally occurring levels, they may be eliminated from the quantitative risk assessment. In some cases, however, background concentrations may present a significant risk, and, while cleanup may or may not eliminate this risk, the background risk may be an important site characteristic to those exposed. The RPM will always have the option to consider the risk posed by naturally occurring background chemicals separately.

In general, comparison with naturally occurring levels is applicable only to inorganic chemicals, because the majority of organic chemicals found at Superfund sites are not naturally occurring (even though they may be ubiquitous). The presence of organic chemicals in background samples collected during a site investigation actually may indicate that the sample was collected in an area influenced by site contamination and therefore does not qualify as a true background sample. Such samples should instead be included with other site samples in the risk assessment. Unless a very strong case can be made for the natural occurrence of an organic chemical, do not eliminate it from the quantitative risk assessment for this reason.

5.7.4 COMPARE CHEMICAL CONCENTRATIONS WITH ANTHROPOGENIC LEVELS

Anthropogenic levels are ambient concentrations resulting from human (non-site) sources. Localized anthropogenic background is often caused by a point source such as a nearby factory. Ubiquitous anthropogenic background is often from nonpoint sources such as automobiles. In general, do not eliminate anthropogenic chemicals because, at many sites, it is extremely difficult to conclusively show at this stage of the site investigation that such chemicals are present at the site due to operations not related to the site or the surrounding area.

Often, anthropogenic background chemicals can be identified and considered separately during or at the end of the risk assessment. These chemicals also can be omitted entirely from the risk assessment, but, as discussed for natural background, they may present a significant risk. Omitting anthropogenic background chemicals

from the risk assessment could result in the loss of important information for those potentially exposed.

5.8 DEVELOPMENT OF A SET OF CHEMICAL DATA AND INFORMATION FOR USE IN THE RISK ASSESSMENT

After the evaluation of data is complete as specified in previous sections, a list of the samples (by medium) is made that will be used to estimate exposure concentrations, as discussed in Chapter 6 of this guidance. In addition, as shown in the flowchart in Exhibit 5-1, a list of chemicals of potential concern (also by medium) will be needed for the quantitative risk assessment. This list should include chemicals that were:

(1) positively detected in at least one CLP sample (RAS or SAS) in a given medium, including (a) chemicals with no qualifiers attached (excluding samples with unusually high detection limits), and (b) chemicals with qualifiers attached that indicate known identities but unknown concentrations (e.g., J-qualified data);

(2) detected at levels significantly elevated above levels of the same chemicals detected in associated blank samples;

(3) detected at levels significantly elevated above naturally occurring levels of the same chemicals;

(4) only tentatively identified but either may be associated with the site based on historical information or have been confirmed by SAS; and/or

(5) transformation products of chemicals demonstrated to be present.

Chemicals that were not detected in samples from a given medium (i.e., non-detects) but that may be present at the site also may be included in the risk assessment if an evaluation of the risks potentially present at the detection limit is desired.

5.9 FURTHER REDUCTION IN THE NUMBER OF CHEMICALS (OPTIONAL)

For certain sites, the list of potentially site-related chemicals remaining after quantitation limits, qualifiers, blank contamination, and background have been evaluated may be lengthy. Carrying a large number of chemicals through a quantitative risk assessment may be complex, and it may consume significant amounts of time and resources. The resulting risk assessment report, with its large, unwieldy tables and text, may be difficult to read and understand, and it may distract from the dominant risks presented by the site. In these cases, the procedures discussed in this section -- using chemical classes, frequency of detection, essential nutrient information, and a concentration-toxicity screen -- may be used to further reduce the number of chemicals of potential concern in each medium.

If conducting a risk assessment on a large number of chemicals is feasible (e.g., because of adequate computer capability), then the procedures presented in this section should not be used. Rather, the most important chemicals (e.g., those presenting 99 percent of the risk) -- identified after the risk assessment -- could be presented in the main text of the report, and the remaining chemicals could be presented in the appendices.

5.9.1 CONDUCT INITIAL ACTIVITIES

Several activities must be conducted before implementing any of the procedures described in this section: (1) consult with the RPM; (2) consider how the rationale for the procedure should be documented; (3) examine historical information on the site; (4) consider concentration and toxicity of the chemicals; (5) examine the mobility, persistence, and bioaccumulation potential of the chemicals; (6) consider special exposure routes; (7) consider the treatability of the chemicals; (8) examine applicable or relevant and appropriate requirements (ARARs); and (9) examine the need for the procedures. These activities are described below.

Consultation with the RPM. If a large number of chemicals are of potential concern at a particular

site, the RPM should be consulted. Approval by the RPM must be obtained prior to the elimination of chemicals based on any of these procedures. The concentration-toxicity screen in particular may be needed only in rare instances.

Documentation of rationale. The rationale for eliminating chemicals from the quantitative risk assessment based on the procedures discussed below must be clearly stated in the risk assessment report. This documentation, and its possible defense at a later date, could be fairly resource-intensive. If a continuing need to justify this step is expected, then any plans to eliminate chemicals should be reconsidered.

Historical information. Chemicals reliably associated with site activities based on historical information generally should not be eliminated from the quantitative risk assessment, even if the results of the procedures given in this section indicate that such an elimination is possible.

Concentration and toxicity. Certain aspects of concentration and toxicity of the chemicals also must be considered prior to eliminating chemicals based on the results of these procedures. For example, before eliminating potentially carcinogenic chemicals, the weight-of-evidence classification should be considered in conjunction with the concentrations detected at the site. It may be practical and conservative to retain a chemical that was detected at low concentrations if that chemical is a Group A carcinogen. (As discussed in detail in Chapter 7, the weight-of-evidence classification is an indication of the quality and quantity of data underlying a chemical's designation as a potential human carcinogen.)

Mobility, persistence, and bioaccumulation. Three factors that must be considered when implementing these procedures are the mobility, persistence, and bioaccumulation of the chemicals. For example, a highly volatile (i.e., mobile) chemical such as benzene, a long-lived (i.e., persistent) chemical such as dioxin, or a readily taken-up and concentrated (i.e., bioaccumulated) chemical such as DDT, probably should remain in the risk assessment. These procedures do not explicitly include a mobility, persistence, or bioaccumulation component, and therefore the risk assessor must pay special attention to these factors.

Special exposure routes. For some chemicals, certain exposure routes need to be considered carefully before using these procedures. For example, some chemicals are highly volatile and may pose a significant inhalation risk due to the home use of contaminated water, particularly for showering. The procedures described in this section may not account for exposure routes such as this.

Treatability. Some chemicals are more difficult to treat than others and as a result should remain as chemicals of potential concern because of their importance during the selection of remedial alternatives.

ARARs. Chemicals with ARARs (including those relevant to land ban compliance) usually are not appropriate for exclusion from the quantitative risk assessment based on the procedures in this section. This may, however, depend in part on how the chemicals' site concentrations in specific media compare with their ARAR concentrations for these media.

Need for procedures. Quantitative evaluation of all chemicals of potential concern is the most thorough approach in a risk assessment. In addition, the time required to implement and defend the selection procedures discussed in this section may exceed the time needed to simply carry all the chemicals of potential concern through the risk assessment. Usually, carrying all chemicals of potential concern through the risk assessment will not be a difficult task, particularly given the widespread use of computer spreadsheets to calculate exposure concentrations of chemicals and their associated risks. Although the tables that result may indeed be large, computer spreadsheets significantly increase the ability to evaluate a number of chemicals in a relatively short period of time. For these reasons, the procedures discussed here may be needed only in rare instances. As previously stated, the approval of these procedures by the RPM must be obtained prior to implementing any of these optional screening procedures at a particular site.

5.9.2 GROUP CHEMICALS BY CLASS

At times, toxicity values to be used in characterizing risks are available only for certain chemicals within a chemical class. For example, of the polycyclic aromatic hydrocarbons (PAHs) considered to be potential carcinogens, a slope factor currently is available (i.e., as this manual went to press) for benz(a)pyrene only. In these cases, rather than eliminating the other chemicals within the class from quantitative evaluation because of a lack of toxicity values, it may be useful to group data for such a class of chemicals (e.g., according to structure-activity relationships or other similarities) for consideration in later sections of the risk assessment. For example, the concentrations of only one group of chemicals (e.g., carcinogenic PAHs) would be considered rather than concentrations of each of the seven carcinogenic PAHs currently on the TCL.

To group chemicals by class, concentrations of chemicals within each class are summed according to procedures discussed in Chapter 6 of this guidance. Later in the risk assessment, this chemical class concentration would be used to characterize risk using toxicity values (i.e., RfDs or slope factors) associated with one of the chemicals in the particular class.

Three notes of caution when grouping chemicals should be considered: (1) do not group solely by toxicity characteristics; (2) do not group all carcinogenic chemicals or all noncarcinogenic chemicals without regard to structure-activity or other chemical similarities; and (3) discuss in the risk assessment report that grouping can produce either over- or under-estimates of the true risk.

5.9.3 EVALUATE FREQUENCY OF DETECTION

Chemicals that are infrequently detected may be artifacts in the data due to sampling, analytical, or other problems, and therefore may not be related to site operations or disposal practices. Consider the chemical as a candidate for elimination from the quantitative risk assessment if: (1) it is detected infrequently in one or perhaps two environmental media, (2) it is not detected in any other sampled media or at high concentrations, and (3) there is no reason to believe that the chemical may be present. Available modeling results may indicate whether monitoring data that show infrequently detected chemicals are representative of only their sampling locations or of broader areas. Because chemical concentrations at a site are spatially variable, the risk assessor can use modeling results to project infrequently detected chemical concentrations over broader areas when determining whether the subject chemicals are relevant to the overall risk assessment. Judicious use of modeling to supplement available monitoring data often can minimize the need for the RPM to resort to arbitrarily setting limits on inclusion of infrequently detected chemicals in the risk assessment. Any detection frequency limit to be used (e.g., five percent) should be approved by the RPM prior to using this screen. If, for example, a frequency of detection limit of five percent is used, then at least 20 samples of a medium would be needed (i.e., one detect in 20 samples equals a five percent frequency of detection).

In addition to available monitoring data and modeling results, the risk assessor will need to consider other relevant factors (e.g., presence of sensitive subpopulations) in recommending appropriate site-specific limits on inclusion of infrequently detected chemicals in the quantitative risk assessment. For example, the risk assessor should consider whether the chemical is expected to be present based on historical data or any other relevant information (e.g., known degradation products of chemicals present at the site, modeling results). Chemicals expected to be present should not be eliminated. (See the example of chemicals with similar transport and fate characteristics in Section 5.3.5.)

The reported or modeled concentrations and locations of chemicals should be examined to check for hotspots, which may be especially important for short-term exposures and which therefore should not be eliminated from the risk assessment. Always consider detection of particular chemicals in all sampled media because some media may be sources of contamination for other media. For example, a chemical that is infrequently detected in soil (a potential ground-water contamination source) probably should not be eliminated as a site

contaminant if the same chemical is frequently detected in ground water. In addition, infrequently detected chemicals with concentrations that greatly exceed reference concentrations should not be eliminated.

5.9.4 EVALUATE ESSENTIAL NUTRIENTS

Chemicals that are (1) essential human nutrients, (2) present at low concentrations (i.e., only slightly elevated above naturally occurring levels), and (3) toxic only at very high doses (i.e., much higher than those that could be associated with contact at the site) need not be considered further in the quantitative risk assessment. Examples of such chemicals are iron, magnesium, calcium, potassium, and sodium.

Prior to eliminating such chemicals from the risk assessment, they must be shown to be present at levels that are not associated with adverse health effects. The determination of acceptable dietary levels for essential nutrients, however, often is very difficult. Literature values concerning acceptable dietary levels may conflict and may change fairly often as new studies are conducted. For example, arsenic -- a potential carcinogen -- is considered by some scientists to be an essential nutrient based on animal experiments; however, acceptable dietary levels are not well known (EPA 1988f). Therefore, arsenic should be retained in the risk assessment, even though it may be an essential nutrient at undefined dietary levels. Another example of a nutrient that is difficult to characterize is sodium. Although an essential element in the diet, certain levels of sodium may be associated with blood pressure effects in some sensitive individuals (although data indicating an association between sodium in drinking water and hypertension are inadequate [EPA 1987]).

Another problem with determining acceptable dietary levels for essential nutrients is that nutrient levels often are presented in the literature as concentrations within the human body (e.g., blood levels). To identify an essential nutrient concentration to be used for comparison with concentrations in a particular medium at a site, blood (or other tissue) levels of the chemical from the literature must be converted to concentrations in the media of concern for the site (e.g., soil, drinking water).

For these reasons, it may not be possible to compare essential nutrient concentrations with site concentrations in order to eliminate essential nutrient chemicals. In general, only essential nutrients present at low concentrations (i.e., only slightly elevated above background) should be eliminated to help ensure that chemicals present at potentially toxic concentrations are evaluated in the quantitative risk assessment.

5.9.5 USE A CONCENTRATION-TOXICITY SCREEN

The objective of this screening procedure is to identify the chemicals in a particular medium that -- based on concentration and toxicity -- are most likely to contribute significantly to risks calculated for exposure scenarios involving that medium, so that the risk assessment is focused on the "most significant" chemicals.

Calculate individual chemical scores. Two of the most important factors when determining the potential effect of including a chemical in the risk assessment are its measured concentrations at the site and its toxicity. Therefore, in this screening procedure, each chemical in a medium is first scored according to its concentration and toxicity to obtain a risk factor (see the box below). Separate scores are calculated for each medium being evaluated.

INDIVIDUAL CHEMICAL SCORES

$$Rij = (C_{ij})(T_{ij})$$

where:

R_{ij} = risk factor for chemical i in medium j;

C_{ij} = concentration of chemical i in medium j; and

T_{ij} = toxicity value for chemical i in medium j (i.e., either the slope factor or 1/RfD).

The units for the risk factor R_{ij} depend on the medium being screened. In general, the absolute units do not matter, as long as units among chemicals in a medium are the same. To be conservative, the concentration used in the above equation should be the maximum detected concentration determined according to procedures discussed in Chapter 6, and toxicity values should be obtained in accordance with the procedures discussed in Chapter 7.

Chemicals without toxicity values cannot be screened using this procedure. Such chemicals should always be discussed in the risk assessment as chemicals of potential concern; they should not be eliminated from the risk assessment. Guidance concerning chemicals without toxicity values is provided in Chapter 7.

For some chemicals, both oral and inhalation toxicity values are available. In these cases, the more conservative toxicity values (i.e., ones yielding the larger risk factor when used in the above equation) usually should be used. If only one exposure route is likely for the medium being evaluated, then the toxicity values corresponding to that exposure route should be used.

Calculate total chemical scores (per medium). Chemical-specific risk factors are summed to obtain the total risk factor for all chemicals of potential concern in a medium (see the box on this page). A separate R_j will be calculated for carcinogenic and noncarcinogenic effects. The ratio of the risk factor for each chemical to the total risk factor (i.e., R_{ij}/R_j) approximates the relative risk for each chemical in medium j.

Eliminate chemicals. After carefully considering the factors discussed previously in this subsection, eliminate from the risk assessment chemicals with R_{ij}/R_j ratios that are very low compared with the ratios of other chemicals in the medium. The RPM may wish to specify a limit for this ratio (e.g., 0.01; a lower fraction would be needed if site risks are expected to be high). A chemical that contributes less than the specified fraction of the total risk factor for each medium would not be considered further in the risk assessment for that medium. Chemicals exceeding the limit would be considered likely to contribute significantly to risks, as calculated in subsequent stages of the risk assessment. This screening procedure could greatly reduce the number of chemicals carried through a risk assessment, because in many cases only a few chemicals contribute significantly to the total risk for a particular medium.

TOTAL CHEMICAL SCORES

$$R_j = R_{1j} + R_{2j} + R_{3j} + \ldots + R_{ij}$$

where

R_j =total risk factor for medium j; and

$R_{1j} + \ldots + R_{ij}$ =risk factors for chemicals 1 through i in medium j.

The risk factors developed in this screening procedure are to be used only for potential reduction of the number of chemicals carried through the risk assessment and have no meaning outside of the context of the screening procedure. They should not be considered as a quantitative measure of a chemical's toxicity or risk or as a substitute for the risk assessment procedures discussed in Chapters 6, 7, and 8 of this guidance.

5.10 SUMMARY AND PRESENTATION OF DATA

The section of the risk assessment report summarizing the results of the data collection and evaluation should be titled "Identification of Chemicals of Potential Concern" (see Chapter 9). Information in this section should be presented in ways that readily support the calculation of exposure concentrations in the exposure assessment portion of the risk assessment. Exhibits 5-6 and 5-7 present examples of tables to be included in this section of the risk assessment report.

EXHIBIT 5-6

EXAMPLE OF TABLE FORMAT FOR PRESENTING CHEMICALS SAMPLED IN SPECIFIC MEDIA

Table X
Chemicals Sampled in Medium Y
(and in Operable Unit Z, if appropriate)
Name of Site, Location of Site

Chemical	Frequency of Detection[a]	Range of Sample Quantitation Limits (units)	Range of Detected Concentrations (units)	Background Levels
Chemical A	3/25	5 - 50	320 - 4600	100 - 140
* Chemical B	25/25	1 - 32	16 - 72	--

-- = Not available.

* Identified as a chemical of potential concern based on evaluation of data according to procedures described in text of report.

[a] Number of samples in which the chemical was positively detected over the number of samples available.

EXHIBIT 5-7

EXAMPLE OF TABLE FORMAT FOR SUMMARIZING CHEMICALS OF POTENTIAL CONCERN IN ALL MEDIA SAMPLED

Table W
Summary of Chemicals of
Potential Concern at Site X, Location Y
(and in Operable Unit Z, if appropriate)

Chemical	Concentration				
	Soils (mg/kg)	Ground Water (ug/L)	Surface Water (ug/L)	Sediments (ug/kg)	Air (ug/m^3)
Chemical A	5 - 1,100	--	2 - 30	--	--
Chemical B	0.5 - 64	5 - 92	--	100 - 45,000	--
Chemical C	--	15 - 890	50 - 11,000	--	--
Chemical D	2 - 12	--	--	--	0.1 - 940

-- = Not available.

5.10.1 SUMMARIZE DATA COLLECTION AND EVALUATION RESULTS IN TEXT

In the introduction for this section of the risk assessment report, clearly discuss in bullet form the steps involved in data evaluation. If the optional screening procedure described in Section 5.9 was used in determining chemicals of potential concern, these steps should be included in the introduction. If both historical data and current data were used in the data evaluation, state this in the introduction. Any special site-specific considerations in collecting and evaluating the data should be mentioned. General uncertainties concerning the quality associated with either the collection or the analysis of samples should be discussed so that the potential effects of these uncertainties on later sections of the risk assessment can be determined.

In the next part of the report, discuss the samples from each medium selected for use in quantitative risk assessment. Provide information concerning the sample collection methods used (e.g., grab, composite) as well as the number and location of samples. If this information is provided in the RI report, simply refer to the appropriate sections. If any samples (e.g., field screening/analytical samples) were excluded specifically from the quantitative risk assessment prior to evaluating the data, document this along with reasons for the exclusion. Again, remember that such samples, while not used in the quantitative risk assessment, may be useful for qualitative discussions and therefore should not be entirely excluded from the risk assessment.

Discuss the data evaluation either by medium, by medium within each operable unit (if the site is sufficiently large to be divided into specific operable units), or by discrete areas within each medium in an operable unit. For each medium, if several source areas with different types and concentrations of chemicals exist, then the medium-specific discussion for each source area may be separate. Begin the discussion with those media (e.g., wastes, soils) that are potential sources of contamination for other media (e.g., ground water, surface water/sediments). If no samples or data were available for a particular medium, discuss this in the text. For soils data, discuss surface soil results separately from those of subsurface soils. Present ground-water results by aquifer if more than one aquifer was sampled. Discuss surface water/sediment results by the specific surface water body sampled.

For each medium, identify in the report the chemicals for which samples were analyzed, and list the analytes that were detected in at least one sample. If any detected chemicals were eliminated from the quantitative risk assessment based on evaluation of data (i.e., based on evaluation of data quality, background comparisons, and the optional screening procedures, if used), provide reasons for the elimination in the text (e.g., chemical was detected in blanks at similar concentrations to those detected in samples or chemical was infrequently detected).

The final subsection of the text is a discussion of general trends in the data results. For example, the text may mention (1) whether concentrations of chemicals of potential concern in most media were close to the detection limits or (2) trends concerning chemicals detected in more than one medium or in more than one operable unit at the site. In addition, the location of hot spots should be discussed, as well as any noticeable trends apparent from sampling results at different times.

5.10.2 SUMMARIZE DATA COLLECTION AND EVALUATION RESULTS IN TABLES AND GRAPHICS

As shown in Exhibit 5-6, a separate table that includes all chemicals detected in a medium can be provided for each medium sampled at a hazardous waste site or for each medium within an operable unit at a site. Chemicals that have been determined to be of potential concern based on the data evaluation should be designated in the table with an asterisk to the left of the chemical name.

For each chemical, present the frequency of detection in a certain medium (i.e., the number of times a chemical was detected over the total number of samples considered) and the range of detected or quantified values in the samples. Do not present the QL or similar indicator of a minimum level (e.g., <10 mg/L, ND) as the lower end of the range; instead, the lower and upper bound of the range should be the minimum and maximum detected values, respectively. The range of reported QLs obtained for each chemical in various samples should be provided

in a separate column. Note that these QLs should be sample-specific; CRQLs, MDLs, or other types of non-sample-specific values should be provided only when SQLs are not available. Note that the range of QLs would not include any limit values (e.g., unusually high QLs) eliminated based on the guidance in Section 5.3. Finally, naturally occurring concentrations of chemicals used in comparing sample concentrations may be provided in a separate column. The source of these naturally occurring levels should be provided in a footnote. List the identity of the samples used in determining concentrations presented in the table in an appropriate footnote.

The final table in this section is a list of the chemicals of potential concern presented by medium at the site or by medium within each operable unit at the site. A sample table format is presented in Exhibit 5-7.

Another useful type of presentation of chemical concentration data is the isopleth (not shown). This graphic characterizes the monitored or modeled concentrations of chemicals at a site and illustrates the spatial pattern of contamination.

ENDNOTE FOR CHAPTER 5

1. Note that the values in this example are for illustration purposes only. Many CRQLs and CRDLs are in the process of being lowered, and the RfDs and slope factors may have changed.

REFERENCES FOR CHAPTER 5

Environmental Protection Agency (EPA). 1984. Methods for Organic Chemical Analysis of Municipal and Industrial Wastewater (EPA 600 Methods) as presented in 40 CFR Part 136, Guidelines Establishing Test Procedures for the Analysis of Pollutants Under the Clean Water Act.

- Used to determine chemicals present in municipal and industrial wastewater as provided under the Clean Water Act. Analytical methods for priority pollutants, including sample preparation, reagents, calibration procedures, QA/QC analytical procedures, and calculations.

Environmental Protection Agency (EPA). 1986. Test Methods for Evaluating Solid Waste (SW-846): Physical/Chemical Methods. Office of Solid Waste.

- Provides analytical procedures to test solid waste to determine if it is a hazardous waste as defined under RCRA. Contains information for collecting solid waste samples and for determining reactivity, corrosivity, ignitability, composition of waste, and mobility of waste components.

Environmental Protection Agency (EPA). 1987. Drinking Water; Proposed Substitution of Contaminants and Proposed List of Additional Substances Which May Require Regulation Under the Safe Drinking Water Act. 52 Federal Register 25720 (July 8, 1987).

Environmental Protection Agency (EPA). 1988a. User's Guide to the Contract Laboratory Program. Office of Emergency and Remedial Response.

- Provides requirements and analytical procedures of the CLP protocols developed from technical caucus recommendations for both organic and inorganic analysis. Contains information on CLP objectives and orientation, CLP structure, description of analytical services, utilization of analytical services, auxiliary support services, and program quality assurance.

Environmental Protection Agency (EPA). 1988b. Contract Laboratory Program Statement of Work for Inorganics Analysis: Multi-media, Multi-concentration. Office of Emergency and Remedial Response. SOW No. 788.

- Provides procedures required by EPA for analyzing hazardous waste disposal site samples (aqueous and solid) for inorganic chemicals (25 elements plus cyanide). Contains analytical, document control, and quality assurance/quality control procedures.

Environmental Protection Agency (EPA). 1988c. Contract Laboratory Program Statement of Work for Organics Analysis: Multi-media, Multi-concentration. Office of Emergency and Remedial Response. SOW No. 288.

- Provides procedures required by EPA for analyzing aqueous and solid hazardous waste samples for 126 volatile, semi-volatile, pesticide, and PCB chemicals. Contains analytical, document control, and quality assurance/quality control procedures.

Environmental Protection Agency (EPA). 1988d. Laboratory Data Validation Functional Guidelines for Evaluating Inorganics Analysis. Office of Emergency and Remedial Response.

- Provides guidance in laboratory data evaluation and validation for hazardous waste site samples analyzed under the EPA CLP program. Aids in determining data problems and shortcomings and potential actions to be taken.

Environmental Protection Agency (EPA). 1988e. Laboratory Data Validation Functional Guidelines for Evaluating Organics Analysis (Functional Guidelines for Organics). Office of Emergency and Remedial Response.

- Provides guidance in laboratory data evaluation and validation for hazardous waste site samples analyzed under the EPA CLP program. Aids in determining data problems and shortcomings and potential actions to be taken.

Environmental Protection Agency (EPA). 1988f. Special Report on Ingested Inorganic Arsenic; Skin Cancer; Nutritional Essentiality. Risk Assessment Forum. EPA 625/3-87/013.

- Technical report concerning the health effects of exposure to ingested arsenic. Includes epidemiologic studies suitable for dose-response evaluation from Taiwan, Mexico, and Germany. Also includes discussions on pathological characteristics and significance of arsenic-induced skin lesions, genotoxicity of arsenic, metabolism and distribution, dose-response estimates for arsenic ingestion and arsenic as an essential nutrient.